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U.S. Army Research, Development and Engineering Command

The CREATIVE Decontamination Performance Evaluation Model

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EDGEWOOD CHEMICAL BIOLOGICAL CENTER
A U.S. Army RDECOM Laboratory

CREATIVE model

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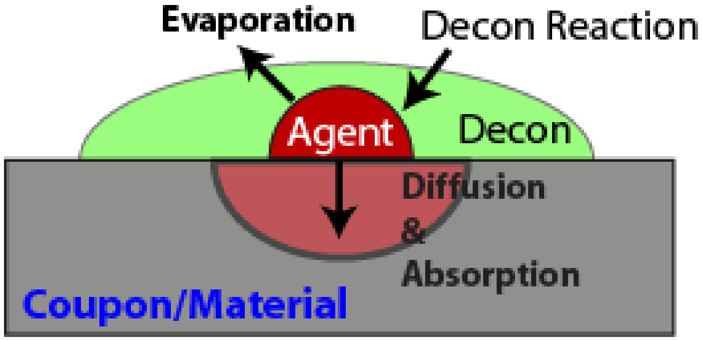
Project Objective

Develop a semi-empirical, deterministic model to characterize and predict *laboratory-scale* decontaminant efficacy and hazards for a range of:

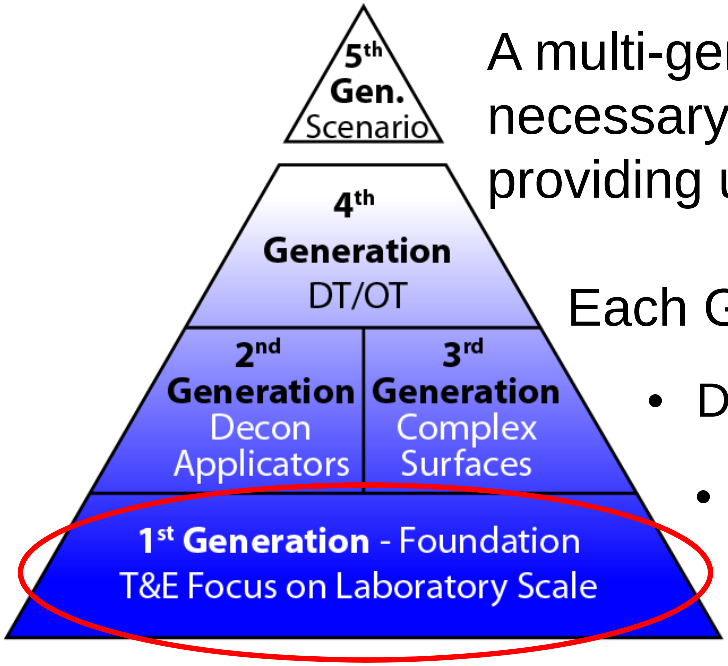
- chemical agents (current focus on HD)
- operational surfaces common to ground vehicle, air craft, equipment construction (e.g., aluminum, glass, CARC, silicone)
- realistic threat challenges (0.5-10 g/m^2)
- environmental conditions (10-40 °C)
- and decontamination process parameters (Decon, residence time).

The model will enable faster characterization of decontaminant performance and provide the capability to predict performance and hazards at untested conditions.



Model Generations

Decontamination is a complex, interacting system. A firm foundation at the laboratory scale is required to understand the perturbations and complexities encountered in the field.



A multi-generation model is proposed to build the necessary tools required to model a full scenario while providing usable tools at each generation stage.

Each Generation provides:

- Distinct value and information.
- Each generation builds upon the foundation adding layers of complexity building towards a full scenario.

This talk applies to the construction of the 1st Generation Foundation Laboratory Model

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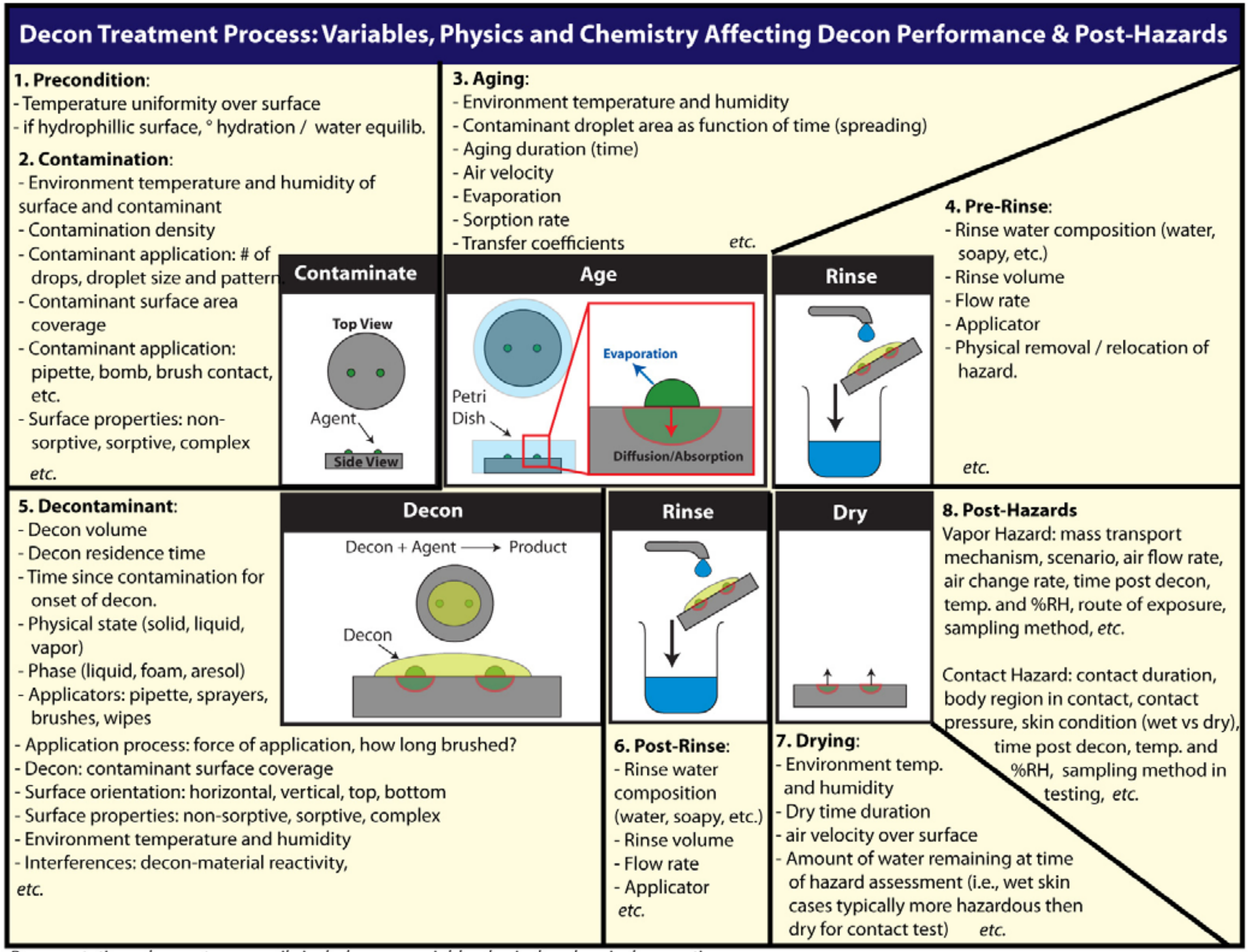
Many Variables Affect Decontamination



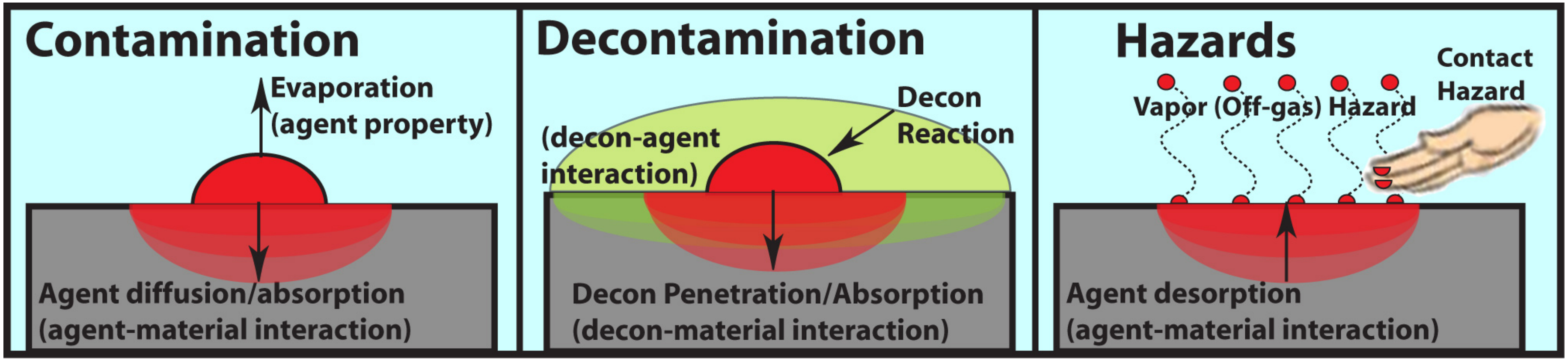
Representation - does not necessarily include every variable, physical or chemical properties.

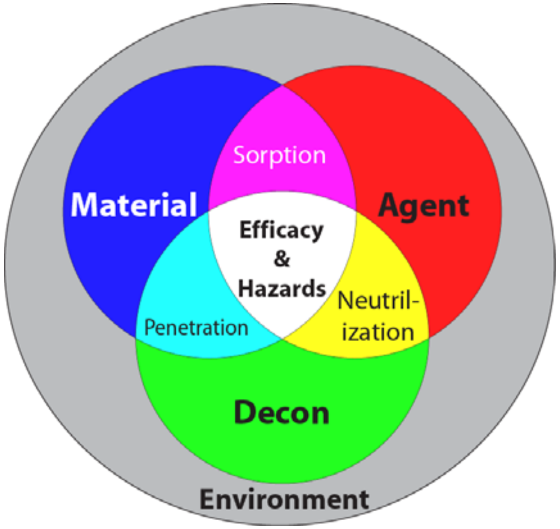
Model construction requires control or measurement of these variables to characterize the core physics representing the model foundation.

Necessary level of control is only available in the laboratory.

As layers of complexity and process steps are introduced data variance and number of variables increase.

Decontamination is Mass Transport



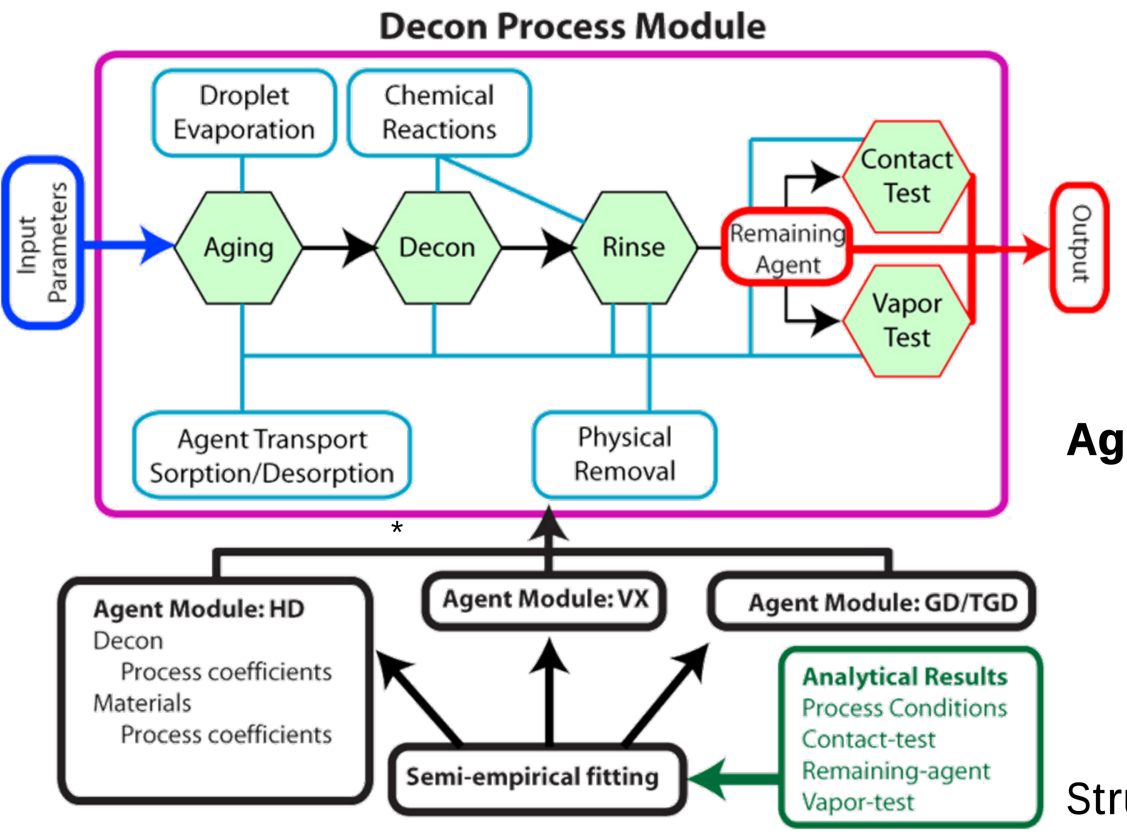


Decontamination testing involves multiple mass transport processes resulting from agent-decon-material interactions:

Material-Agent:	sorption
Decon-Agent:	neutralization/solubility
Decon-Material:	decon penetration
Environment:	alters reaction rates and transport rates.

Post-decon hazards result from mass transport of agent from the surface that may be presented to unprotected personnel.

Module-Based Model Architecture



Decon process module

- Contains mass transport & physics of decon
- Component modules correspond to decon process steps
- Mass transport & physics are similar between agent-material-decons, difference is coefficients

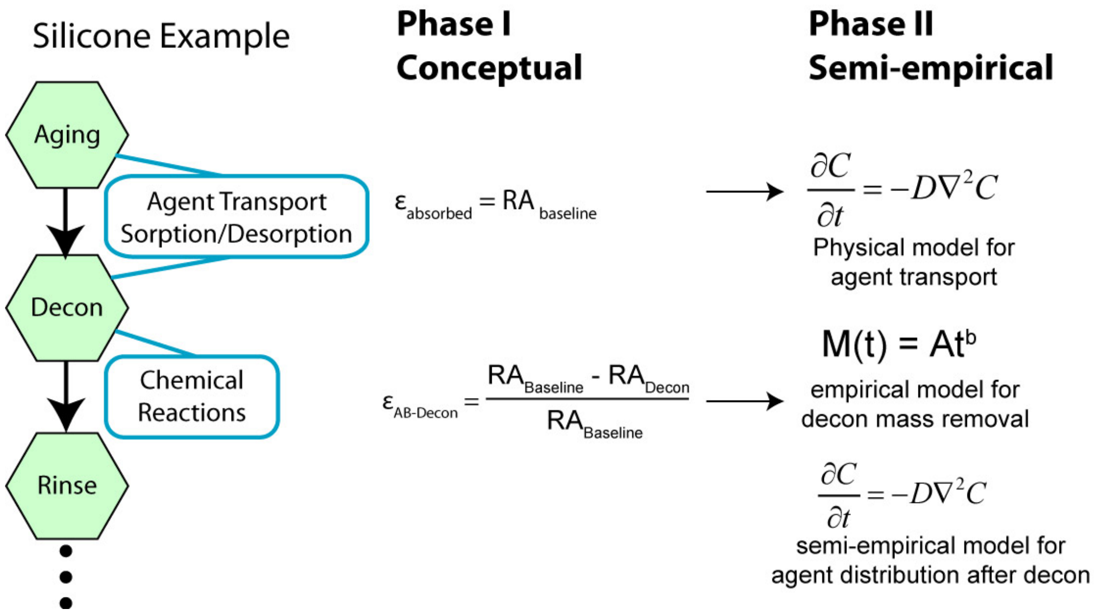
Agent modules

- provide agent-material-decon specific process coefficients
- Semi-empirical methods calculate coefficients from high-quality test data

Structure enables future expansion of agents, materials* and decons without full rebuild of model

*different mass transport mechanisms (e.g., porous transport) may require further model/module development

Model Development



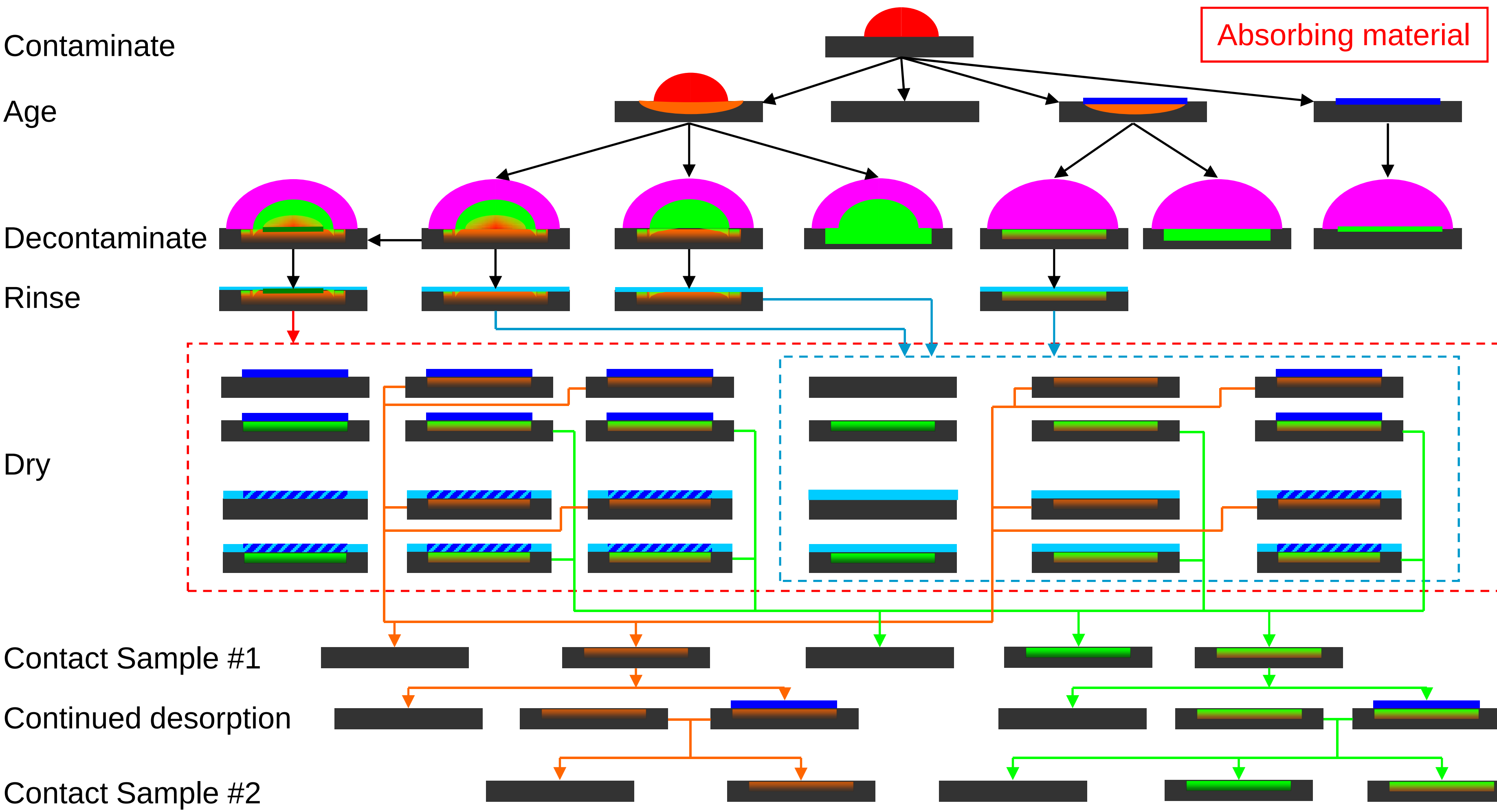
Phase I – Conceptual Model

- Construct full model using empirical relationships and logical assumptions.
- Coefficients are determined from laboratory data
- Modular structure allows individual replacement of process algorithms.
- Conceptual model provides full model execution for limited data set.

Phase II – Physical Model

- Empirical modules are replaced by algorithms based on 1st principles physics and chemistry increasing capability for prediction
- Model retains some empirical elements to account for inadequacies in the physical model or difficulty in measurement of physical variables.

Conceptual Model Covers Range of Responses



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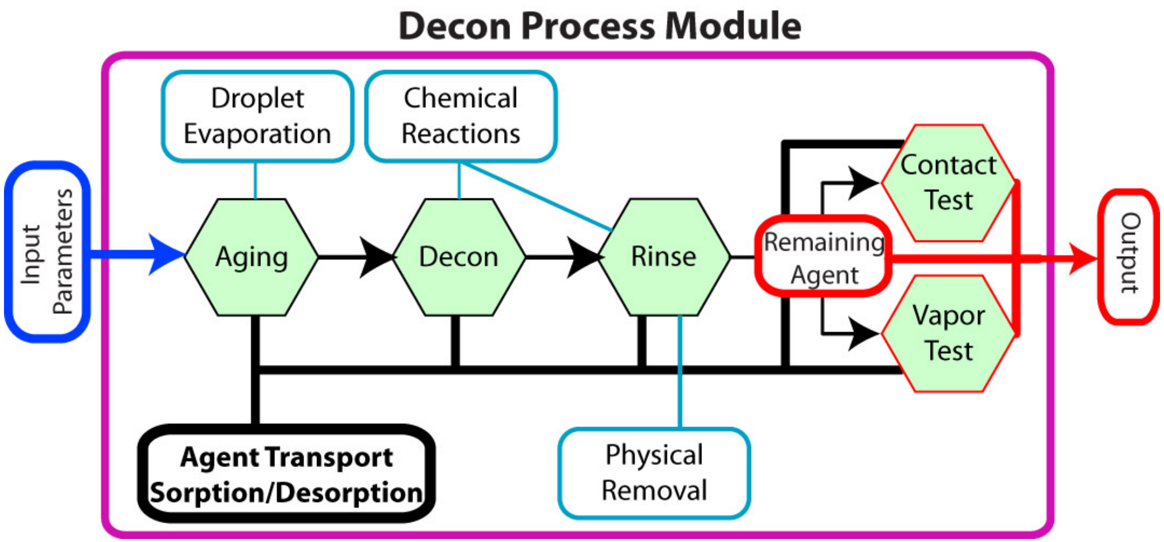
Agent Transport is Core to Decon Testing



Agent transport is determined by material properties and agent-material interactions.

Two questions to answer:

1. How much agent mass sorbed?
   - Determines how much agent to be decontaminated.
2. Where is the agent in the material?
   - Does decon penetrate to same depth to remove agent?
   - Required to predict post-decon hazards.

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Agent Transport Mechanisms

Material properties and agent-material interactions determine mass transport mechanism

Non-porous sorptive transport:

Fick's Second Law (molecular diffusion based)

$$\frac{\partial C}{\partial t} = -D\nabla^2 C = -D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

Most work in literature is for 1D;
1D models are used as a reality check (validation) for the 3D model.

Porous transport:

Darcy's Law (fluid flow through porous materials – e.g., 'wicking')

Many forms in literature; application to CREATIVE under study

Some Relevant Reference Sources:

1. Crank, J., "The Mathematics of Diffusion", Oxford Science Publications
2. Smith, G.D., "Numerical Solution of Partial Differential Equations", University Press
3. Sidman, K.R., *et al*, "Absorption and Desorption of Organic Liquids by Paint Film", ARCLS-CR-82034
4. Philpot, E.F., *et al*, "Model to Describe Penetration of Skin by Sorbed Liquids by Contact", CRDEC-CR-87100
5. Clarke, A., "Spreading and Imbibition of Liquid Drops on Porous Surfaces", Langmuir 2002, 18, 2980
6. Savage *et al*, "Environmental fate of chemical agents: Final Report" ECBC-TR-532, 2007

Finite Difference: Fick's 2nd Law

Finite Difference Solution (using Taylor's series expansion):

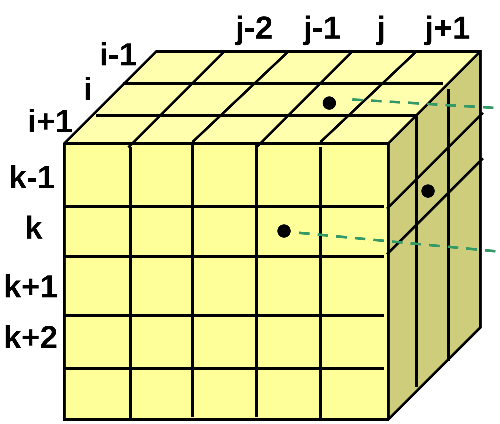
$$C_{i,j,k,t+1} = [\,1 - 2D(r_x + r_y + r_z)]\, C_{i,j,k,t} + Dr_x(C_{i+1,j,k,t} + C_{i-1,j.k.t}) +$$

$$Dr_y(C_{i,j+1,k,t} + C_{i,j-1.k.t}) + Dr_z(C_{i,j,k+1,t} + C_{i,j.k-1.t})$$

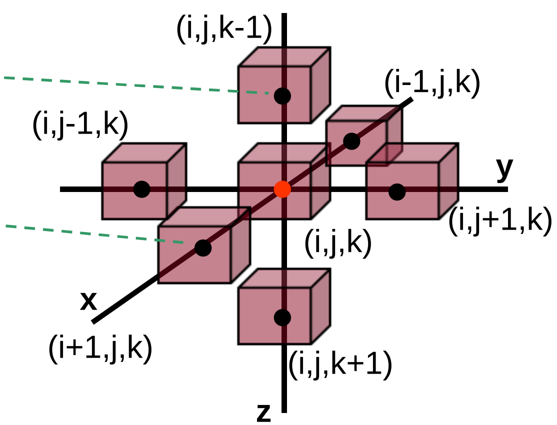
C @ next time step

$$r_n = \frac{\delta t}{\delta n^2} \qquad n = x, y, z$$

For $\delta x = \delta y$ and $\delta z = f \bullet \delta x$ $\qquad \delta t \le \dfrac{\delta x^2}{2\,D\,(\,2 + 1/f^2)}$



Coupon grid elements



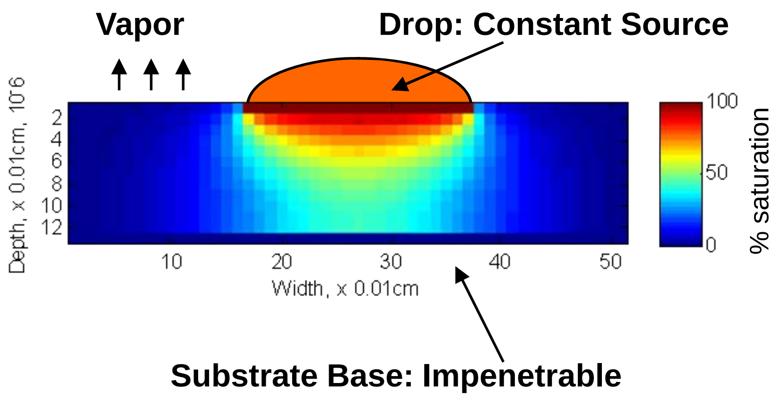
Finite element filter

C = concentration
D = diffusivity
t = time
i.j.k = coordinates
δt = time step
δn = spacing in n direction

Finite Difference Application

Absorption boundary conditions: finite difference equation is altered at boundaries:

1) Drop: constant source until drop disappears
2) Base of substrate considered impenetrable
3) Sides and top of coupon allow mass to escape: rate must be determined



Variables and their sources:

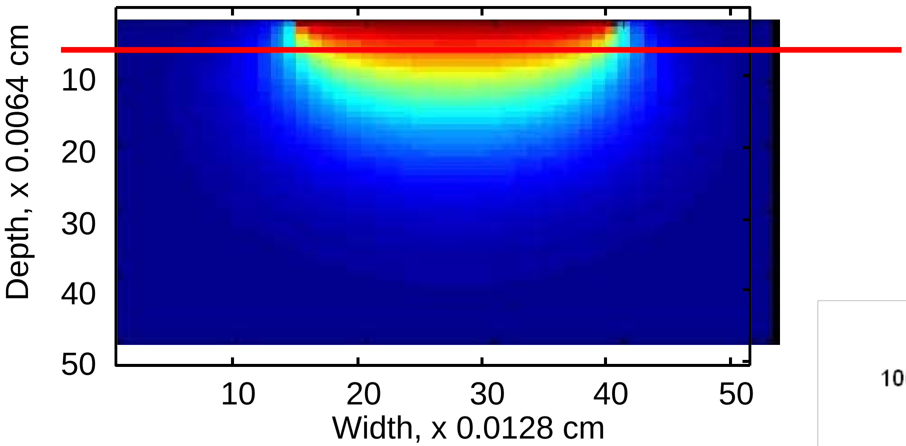
- Diffusivity: literature*
- Saturation Concentration: literature*
- Substrate / Vapor Boundary parameter: CREATIVE (semi-empirically derived)
- Contact boundary parameters: CREATIVE (semi-empirically derived)
- Validation: CREATIVE

* Values may be refined based on CREATIVE results

Finite Difference Advantages:

- Allows modeling of agent distribution in substrate **(critical)**
- Allows perimeter effects including drop spreading or shrinking
- Allows calculations for asymmetric or irregularly shaped drops
- Easily adapted to other sorption approaches, e.g., Darcy's law

Modeling Agent Sorption into Silicone



HD / Silicone

60 min

D: 16×10^{-7} cm²/s

C_o: 90,000 µg/cm³

f1: 0.75

$\delta x, \delta y$: 0.0128 cm

δz: 0.0064 cm

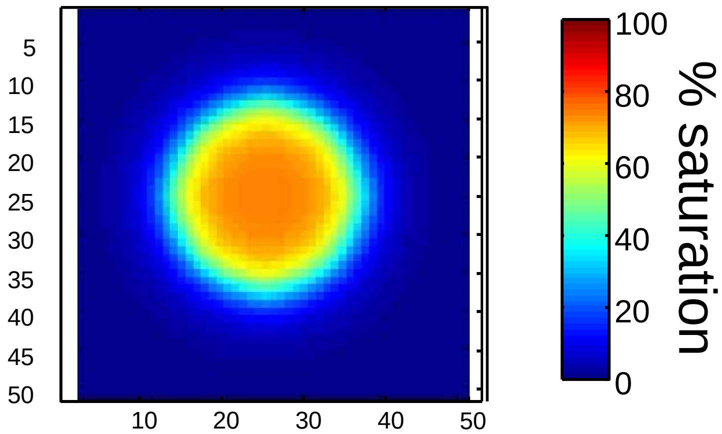
Calculated

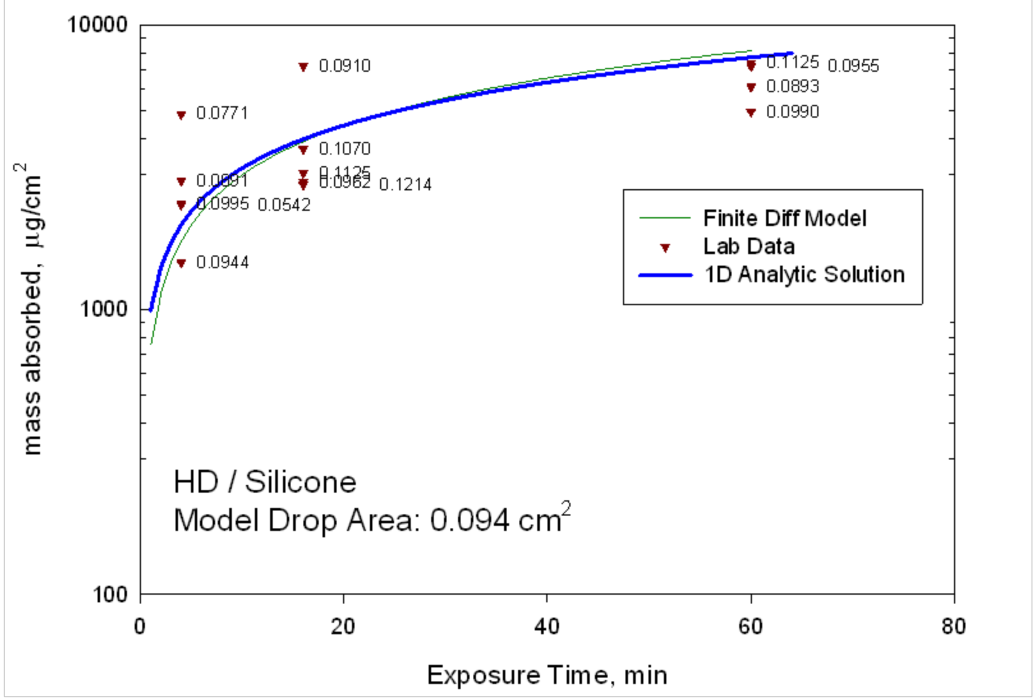
δt: 8.533 s

r_x 0.0833

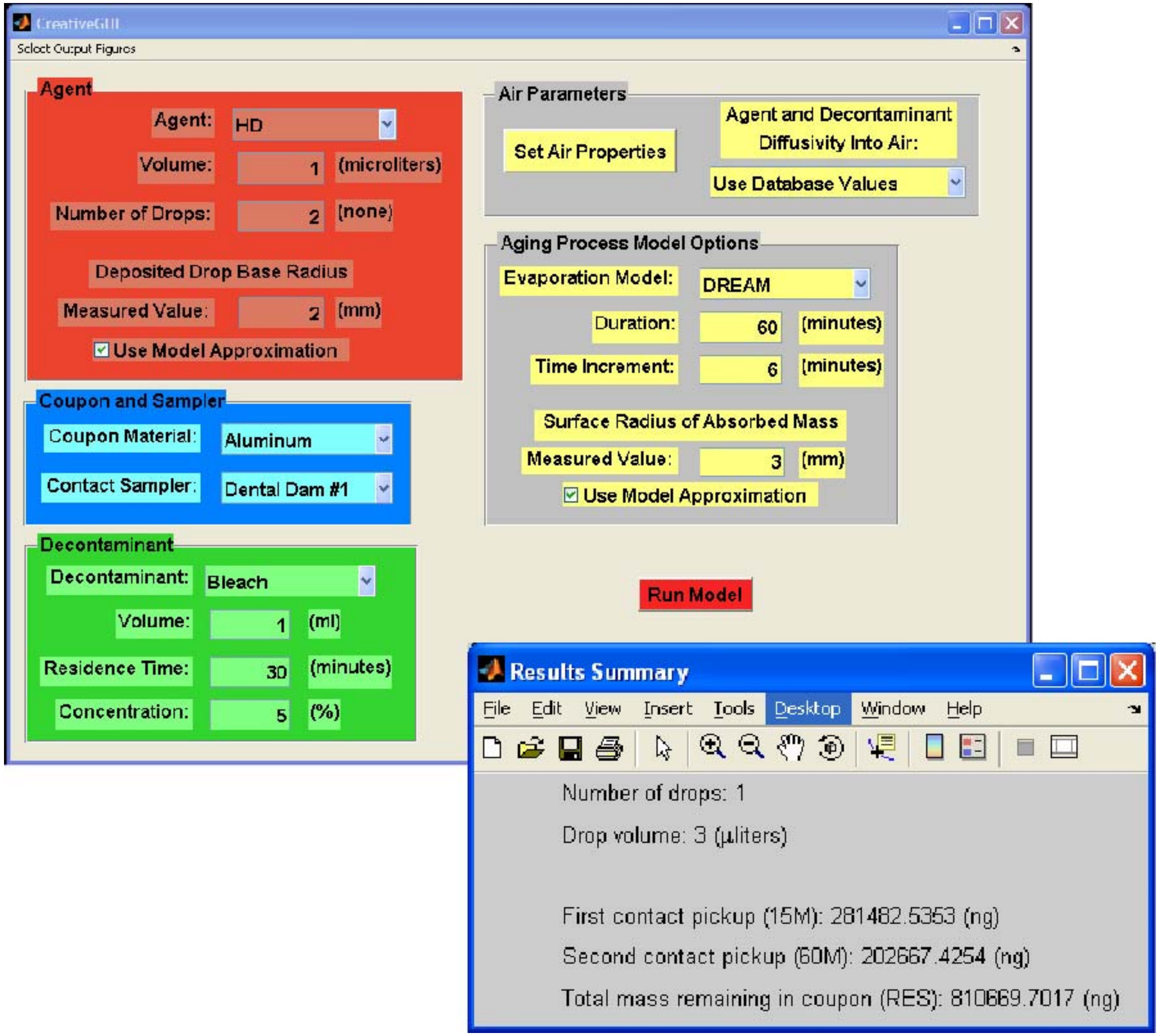
r_y: 0.8333

r_z: 0.3333





1st Generation Interim Model Status



Capabilities

- Models HD on aluminum, glass, and silicone
- Decontaminants include none (baseline), DF200, and bleach
- Data output for contact test, vapor test, and residual agent
- Model developed in Matlab
- GUI interface to input conditions and get response

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Summary and Future Directions

- CREATIVE will enable reduced testing at the laboratory scale to evaluate a decontaminant
- Objective is to predict contact- and vapor-hazards and residual agent
- Implementation of 3D mass transport modeling required to simulate contamination, decontamination, and prediction of hazards
- Agent modules enable future incorporation of new agents, materials, and decons
- Implementation of physical model for agent transport processes enables more confident prediction (and extrapolation) of post-decon hazards
- Approach developed to use indirect characterization of decontamination efficacy in the material to build semi-empirical decon model
- This model provides the laboratory-scale foundation for simulating decontamination efficacy and hazards
- Development of multi-generation approach to mature model to DT/OT and beyond (FY09)

Acknowledgements

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OMI – Dr. Roger Davis, Mike Dunkel

Questions?

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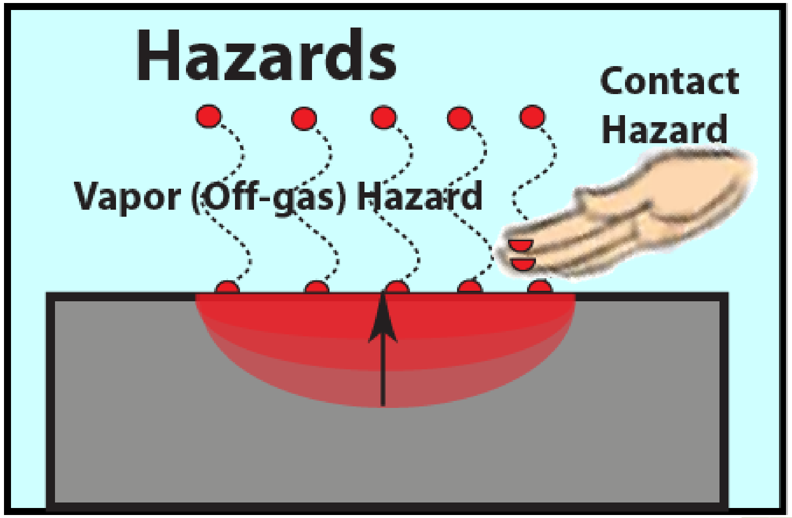
Backups

Decon Performance and Hazards

Decontaminants are evaluated by Performance or Hazards.

Decontaminant: material or process with the ability to reduce a hazard by neutralization or physical removal from the surface of interest.

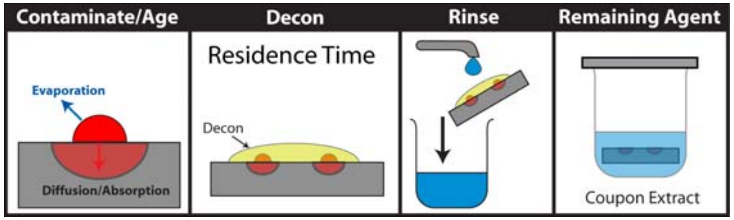


Performance:	How much agent is left.
Hazard:	How much agent presented to unprotected personnel. Hazards are a result of agent transported to or present at the surface after decontamination.
Contact Hazard:	How much agent absorbed by touching surface.
Vapor Hazard:	What vapor concentration generated by material.
Residual Agent:	Mass of agent remaining in test material.

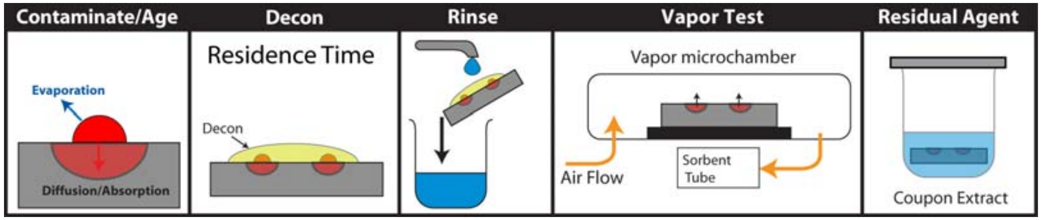
Decon Testing

Three primary tests, defined in the 2007 Source Document, are used to answer :

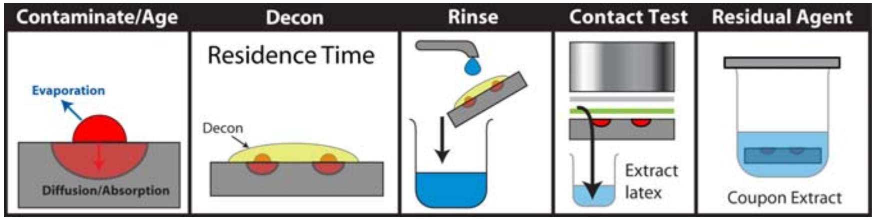
Remaining Agent: how much agent in material.



Vapor Test: vapor emission rate, mass transport out of material (indirect agent distribution)

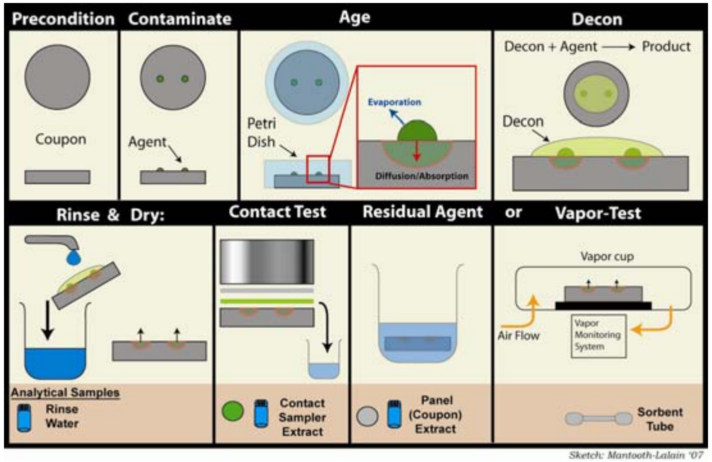


Contact Test: mass of agent transferred to contact sampler, (indirect agent distribution)



Process isolation tests are used to determine the impact and mass transport processes involved in each decontamination process step.

Decontaminant Testing Methods



Methods defined in the 2007 Chemical Decontamination Source Document.

Testing is performed in a high-fidelity laboratory optimized for high-throughput decontamination testing.

Laboratory philosophy: *everything that can be controlled is, everything else is measured*.

Laboratory operates under supervision of a quality manager and is pursuing the implementation of an ISO-17025 quality system.

Analytical uses GC-MSD for HD with detection limits below current acquisition program requirements.

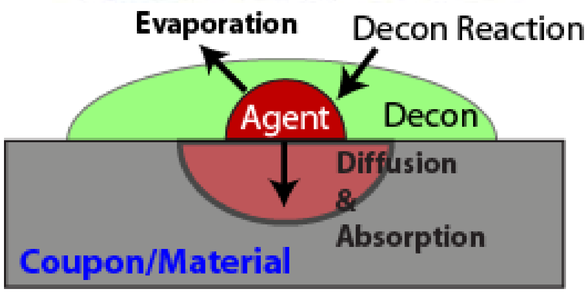
Confidence in laboratory data key for construction of semi-empirical model

- A minimum of 5 sample replicates are acquired for each set point
- Sample replicates are split across multiple days to capture day-to-day variations and prevent artificial trends

Evaluating a Decontaminant

Modeling the panel test with various process conditions provides data that can be used for many applications and answer many questions.

Material + Agent + Contamination + Age Time + Decon + Decon Residence Time + Env. Conditions T / RH = Vapor-Hazard, Contact-Hazard, Residual Agent



Model can be thought of as an algebraic formula

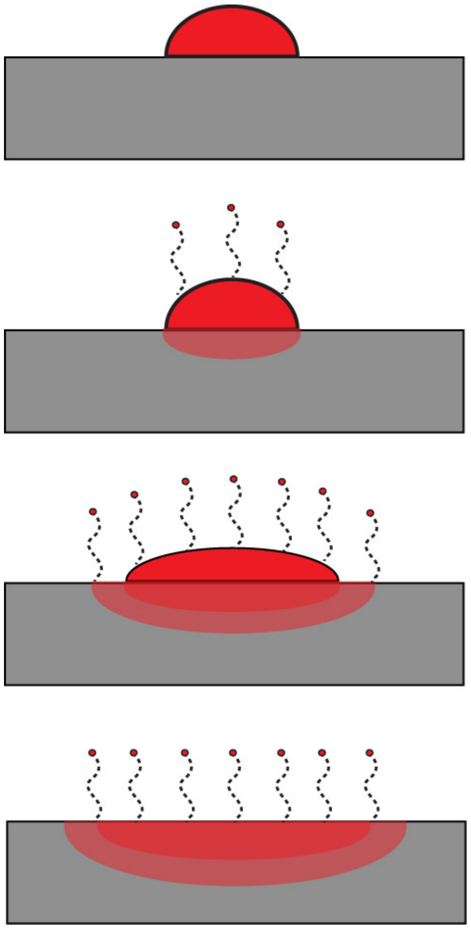
Future work could ‘rearrange’ the equation to solve for any variable such as how long of a decon residence time to reach a requirement.

Keep this slide?? Move??

Currently model answers specific question:

Predict the post-decon hazards of emerging decontaminants to reduce the number of experiments required for evaluation.

Contamination Processes to Model



Processes During Aging:

Sessile droplet evaporation
- Sessile droplet mass tracked to terminate sorption processes.

Sorption
- Dependent on material-agent interactions
  - Agent may be aBsorbed or aDsorbed
- Sorbed agent may evaporate
- Properties of material may require consideration of boundary conditions (e.g., thickness of paint)

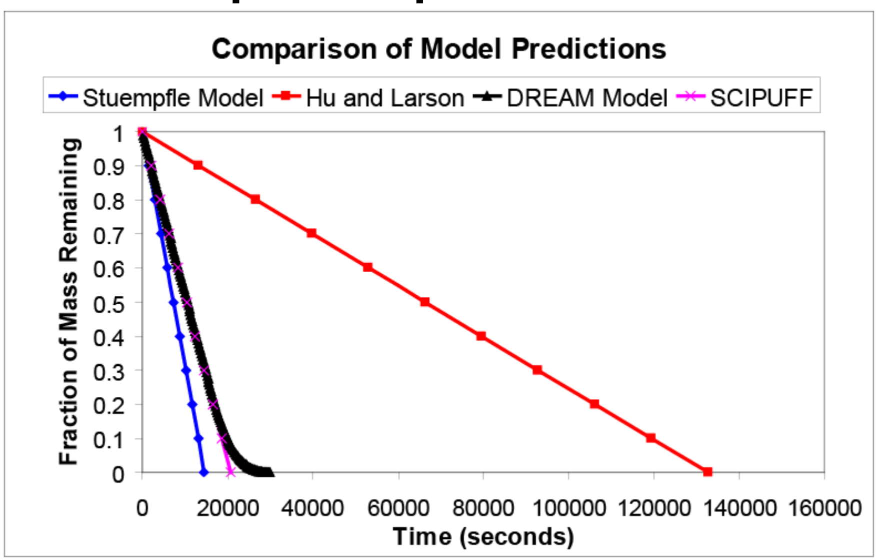
Spreading
- Initially determines droplet contact area
- Material properties and interactions may invoke spreading changing contact area

Existing Models Applicable to System

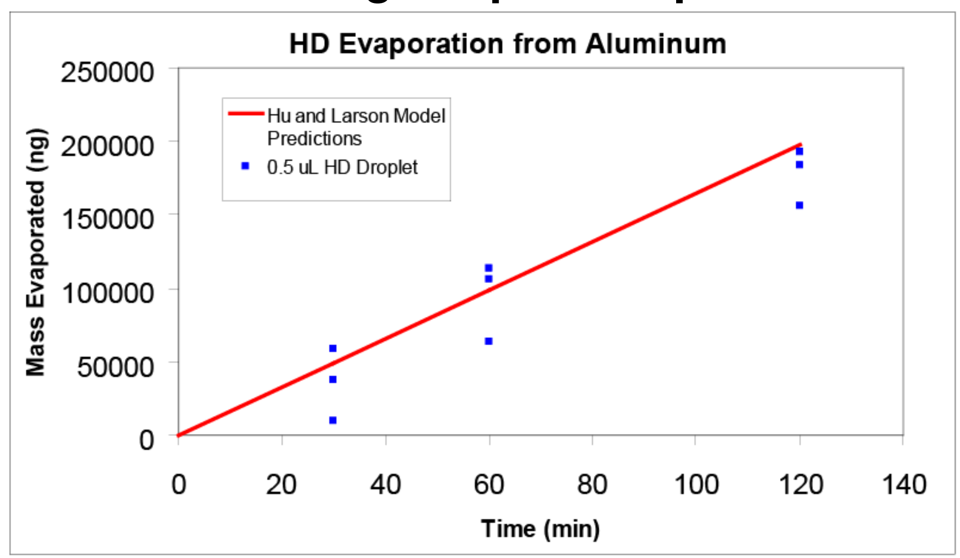
Integrate existing models where available and ensure that assumptions are appropriate for this system.

Hu and Larson model assumes zero air flow.
Appropriate for test conditions.

Droplet Evaporation Models



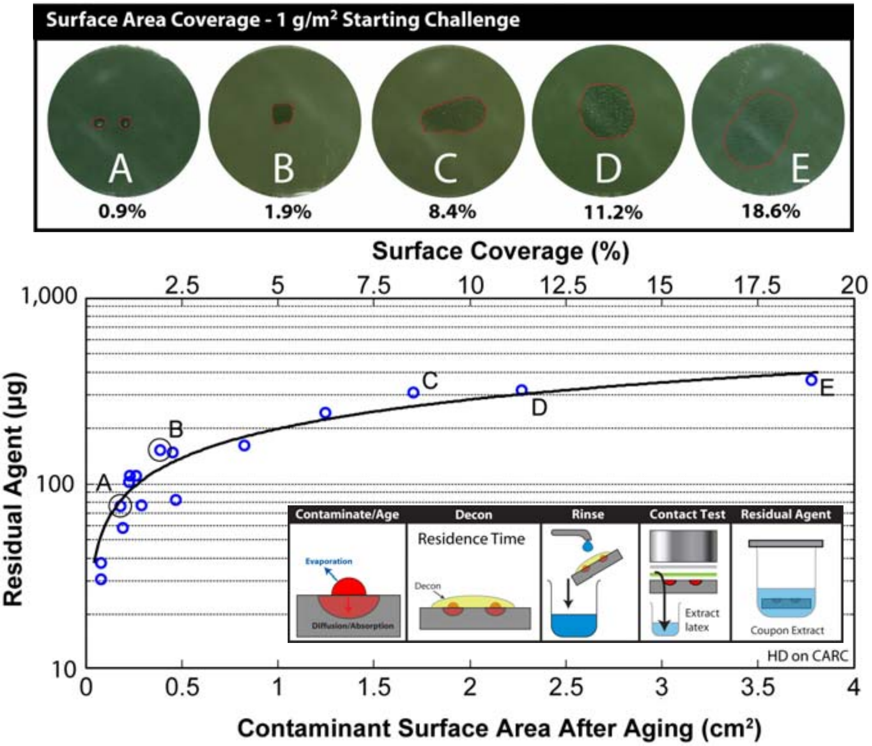
Modeling Droplet Evaporation



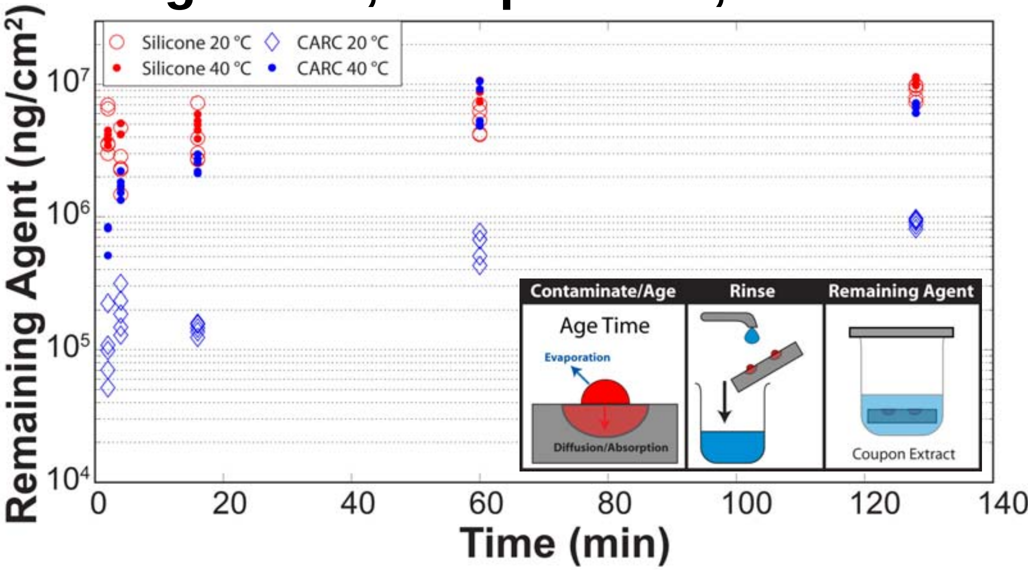
Hu; Larson, *J. Phys. Chem. B.* **106**, 1334 (2002)

Impact of Contamination Variables

Surface Coverage



Age Time, Temperature, Material

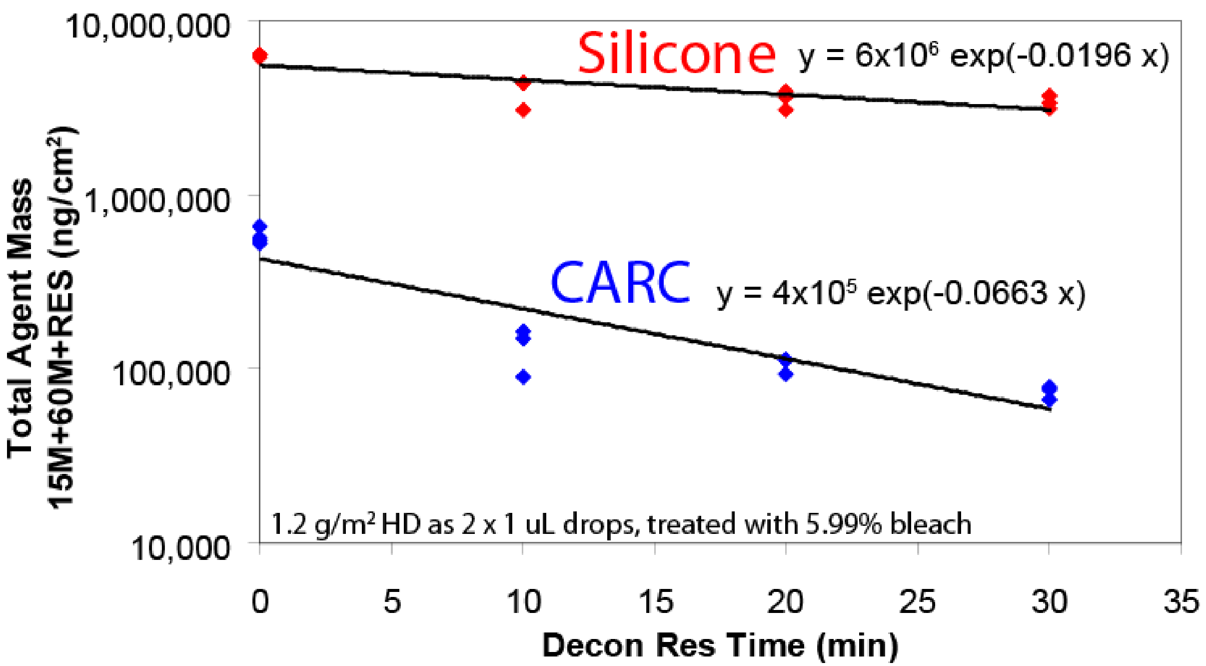


All data points (on right graph) represent 1 x 1 µL drops (0.6 g/m²) HD

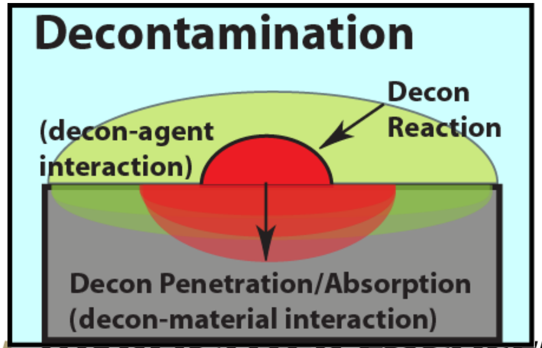
The contaminated surface area, age time, temperature and material contribute to the mass of agent absorbed and its distribution in the material.

The ability of a decontaminant to neutralize/remove agent is dependent on:

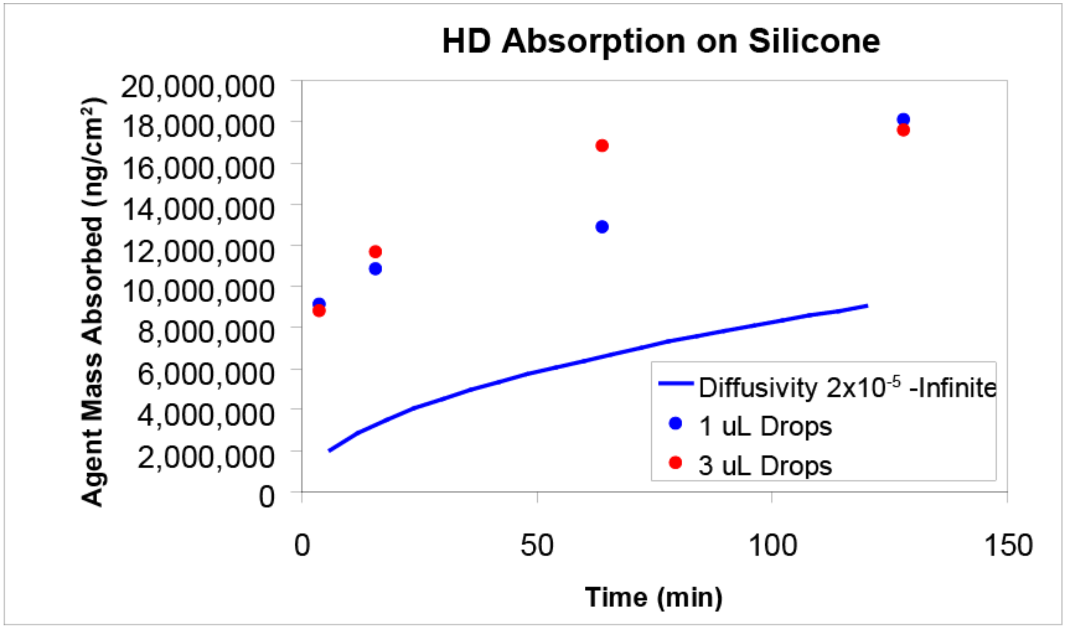
- Decon reaction kinetics – rate of neutralization (usually 1st order exponential).
- Ability to reach agent in material (penetration) determined by material-decon interactions.



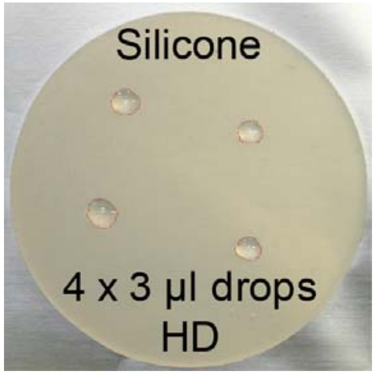
Total agent mass vs. decon residence time shows convolution of decon penetration and reaction kinetics.



Challenges in Absorption Modeling

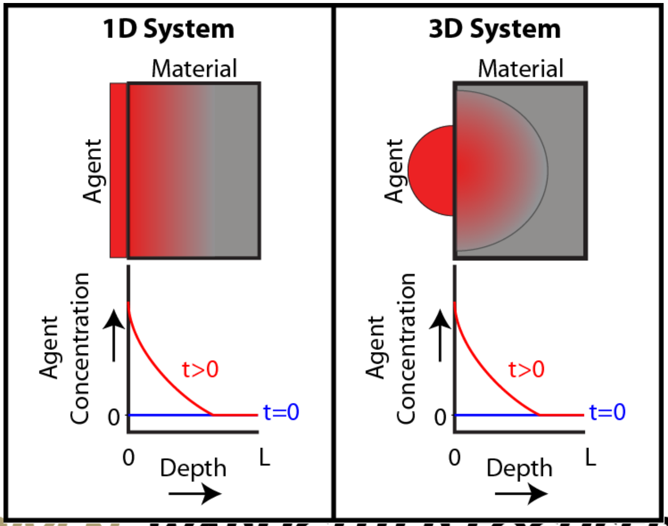


- Most techniques developed in the literature address 1D absorption of a uniform thin film.
- Discrete droplet absorption likely requires modeling 3D absorption.
- Currently investigating finite element and Monte Carlo approaches.



$$C(x,t) = C_0 erfc\left(\frac{x}{2\sqrt{Dt}}\right)$$

Sidman *et. al.*,
ARCSL-CR-82034 (1982)



Process Isolation: Rinse

Each process step contributes towards efficacy and hazards.

Tests are executed to quantify contribution of each step to the system.

Rinse process alone may physically remove all agent.

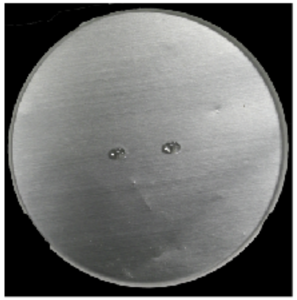
Effect is dependent on agent-material interactions.

Material	Contamination	Decon	15M / 60M / RES
Glass	8 x 2 µL Drops (10 g/m^2)	Rinse only	Below Detection*
	2 x 0.5 µL Drops (0.63 g/m^2)		
Aluminum	8 x 2 µL Drops (10 g/m^2)	Rinse only	Below Detection*
	2 x 0.5 µL Drops (0.63 g/m^2)		

* Quant limit of 40 ng (0.02 mg/m^2)

8 x 2 µL Drops HD on Aluminum

2 x 0.5 µL Drops HD on Aluminum

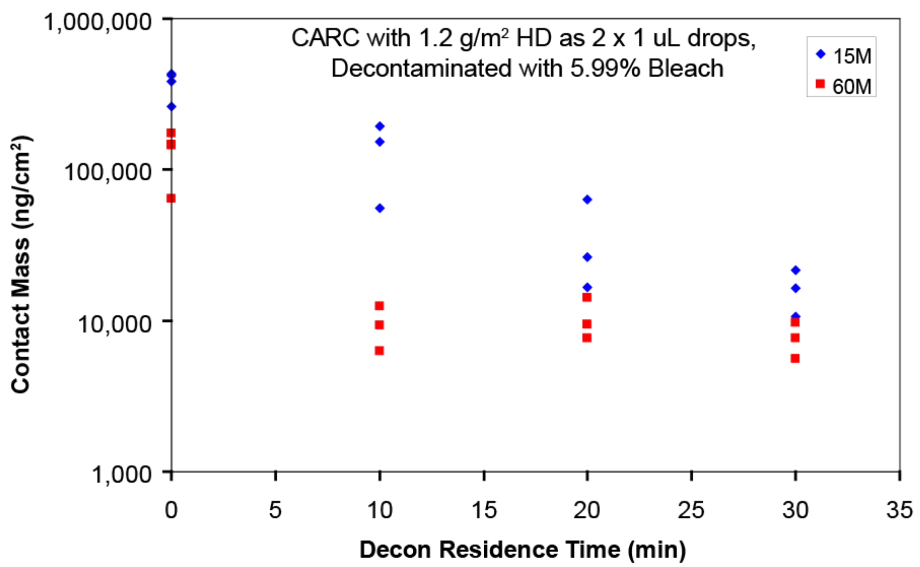


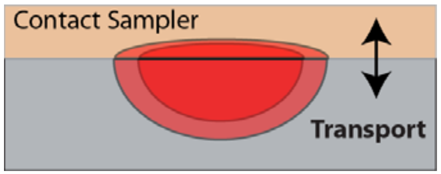
2 x 0.5 µL Drops HD on Glass

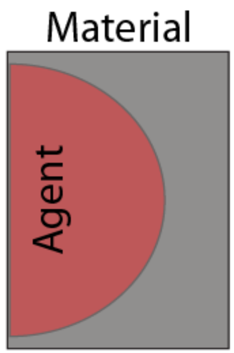
Contact Hazards & Agent Distribution

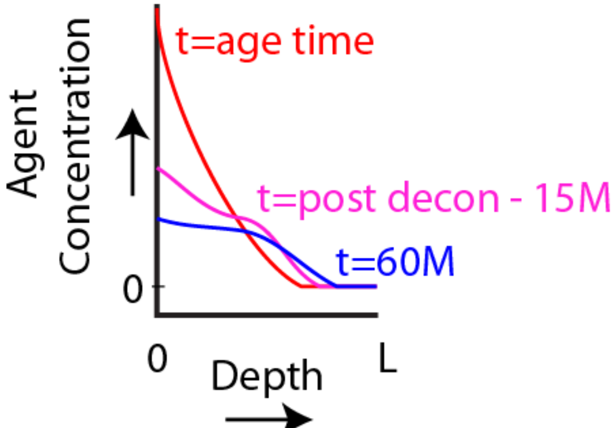
Multiple 'touches' are performed for contact test

- Touch defined as contact sampler in contact with surface for 15 minutes.
- First Touch (15M) starts 15 minutes after rinse – samples top surface of material.
- Second Touch (60M) starts 60 minutes after rinse – samples 'deeper' agent concentration.
- Need to model agent concentration profile to predict hazards.







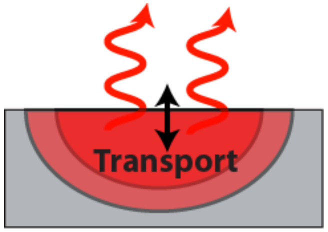


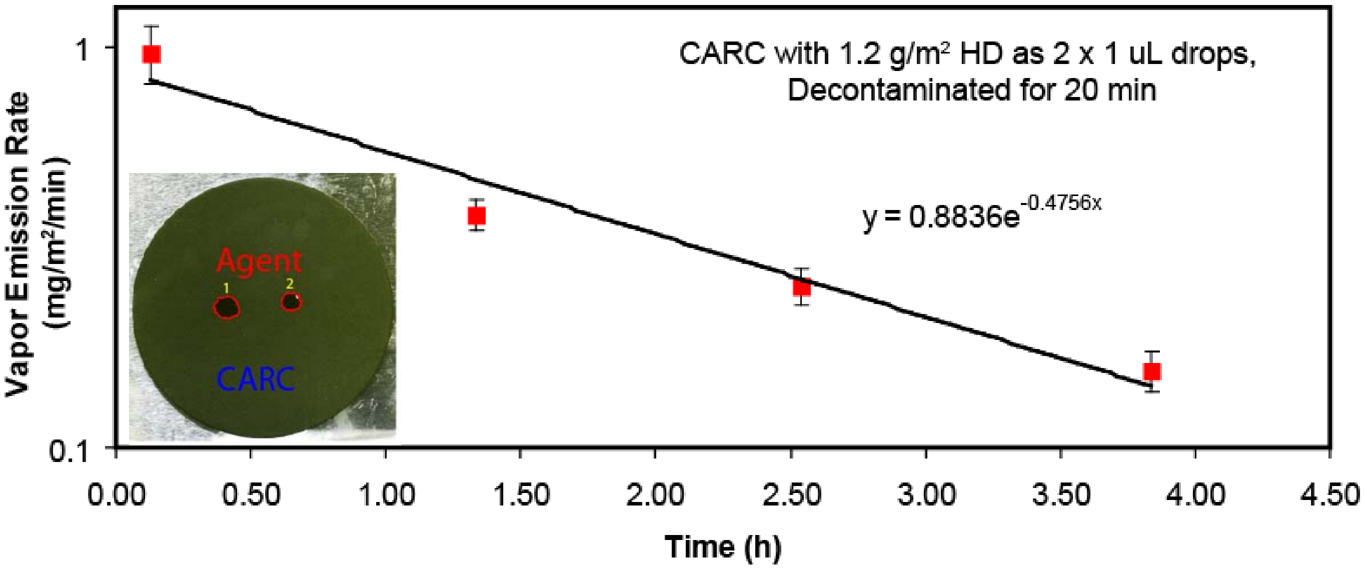
Vapor Emission Rates

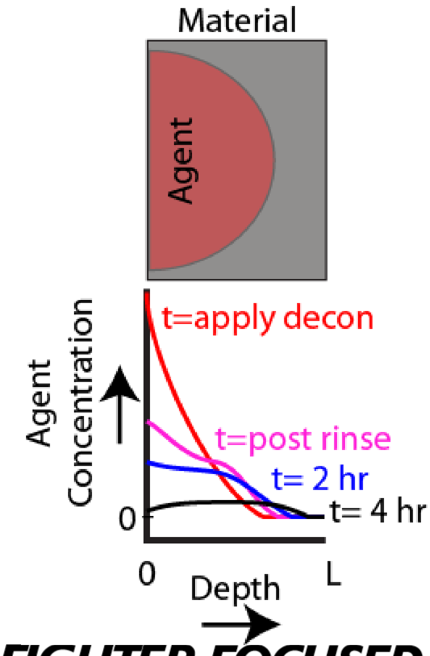
Vapor concentration measured in small-scale vapor chamber enabling vapor emission rate calculation.

Vapor emission rate is a function of mass transport and agent concentration profile in material.

Emission rates can be used to approximate agent distribution in a material to estimate decon penetration.



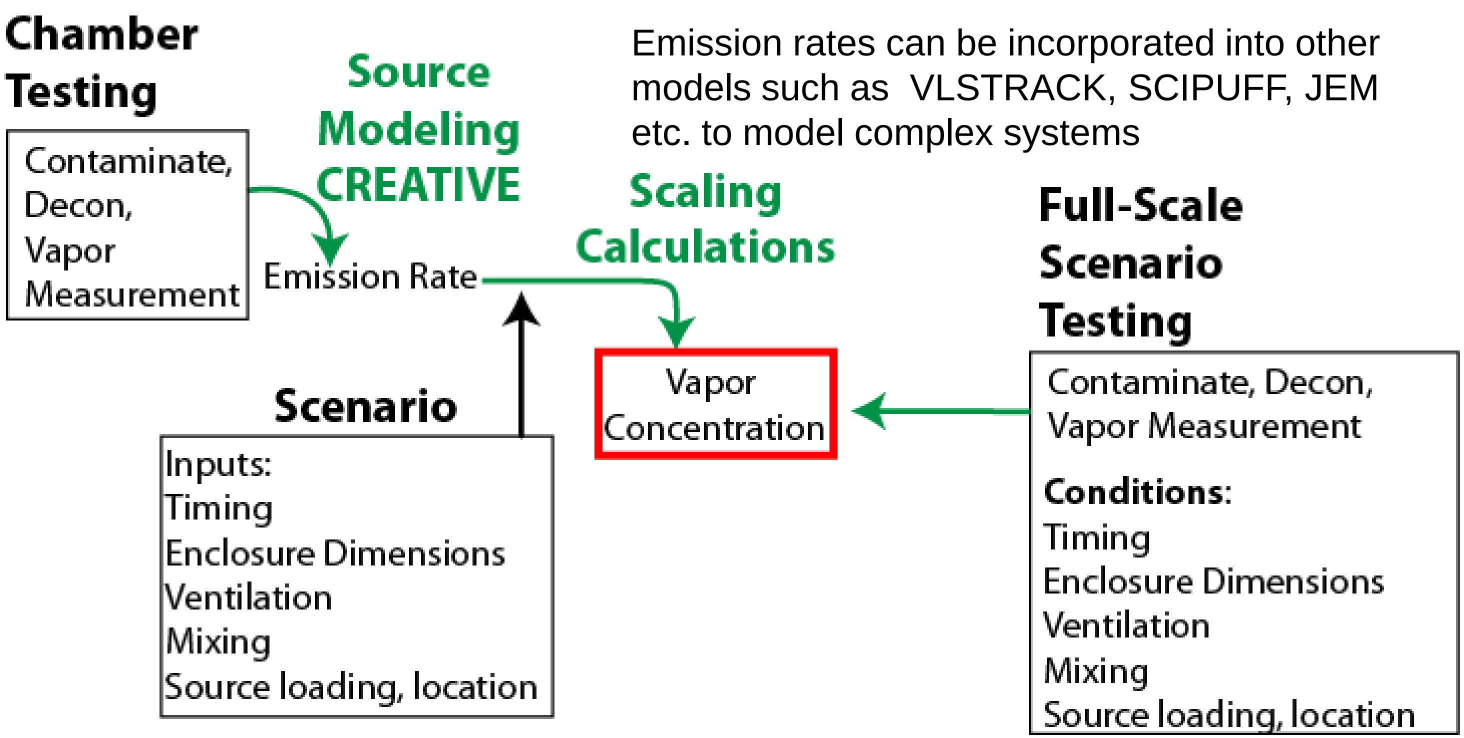




US ARMY RDECOM

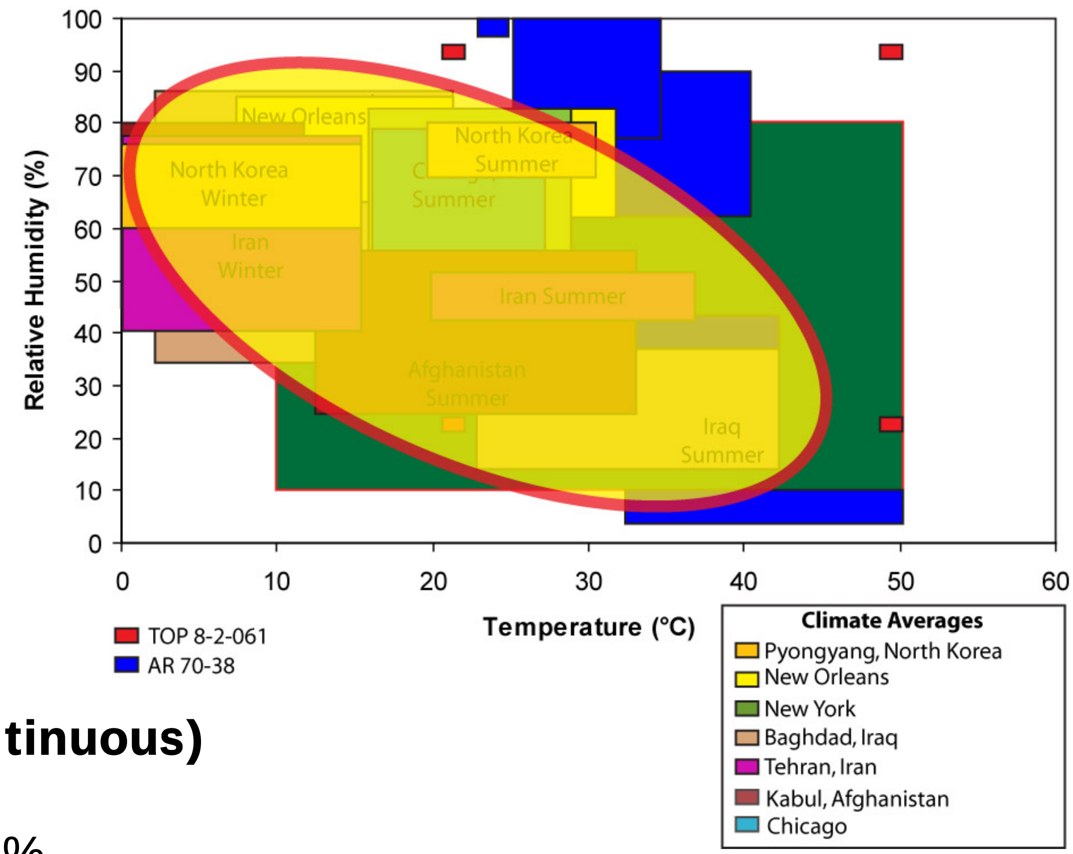
Scaling Lab Data to a Full-Scale Scenario

Using the vapor emission rate of the lab-scale tests modeled in CREATIVE, vapor concentrations can be calculated for full-scale scenarios with simple scaling calculations.



Environmental Conditions

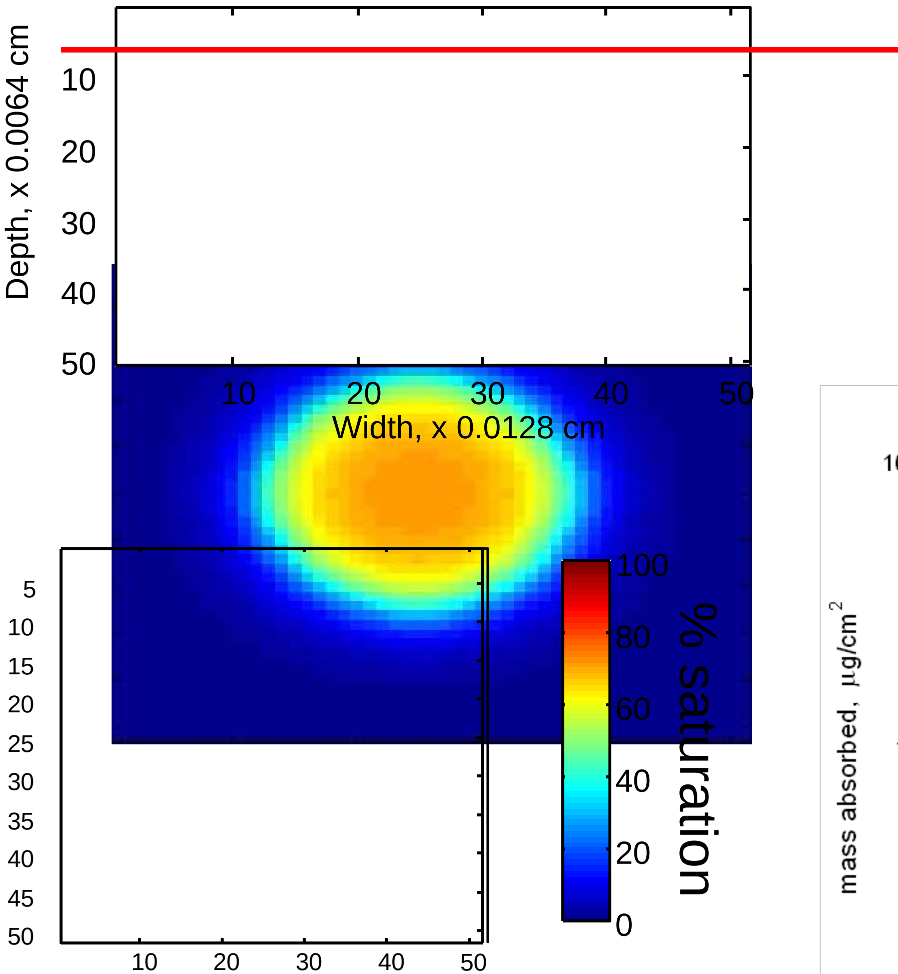
Temperature will affect all mass transport and chemical reaction kinetics.

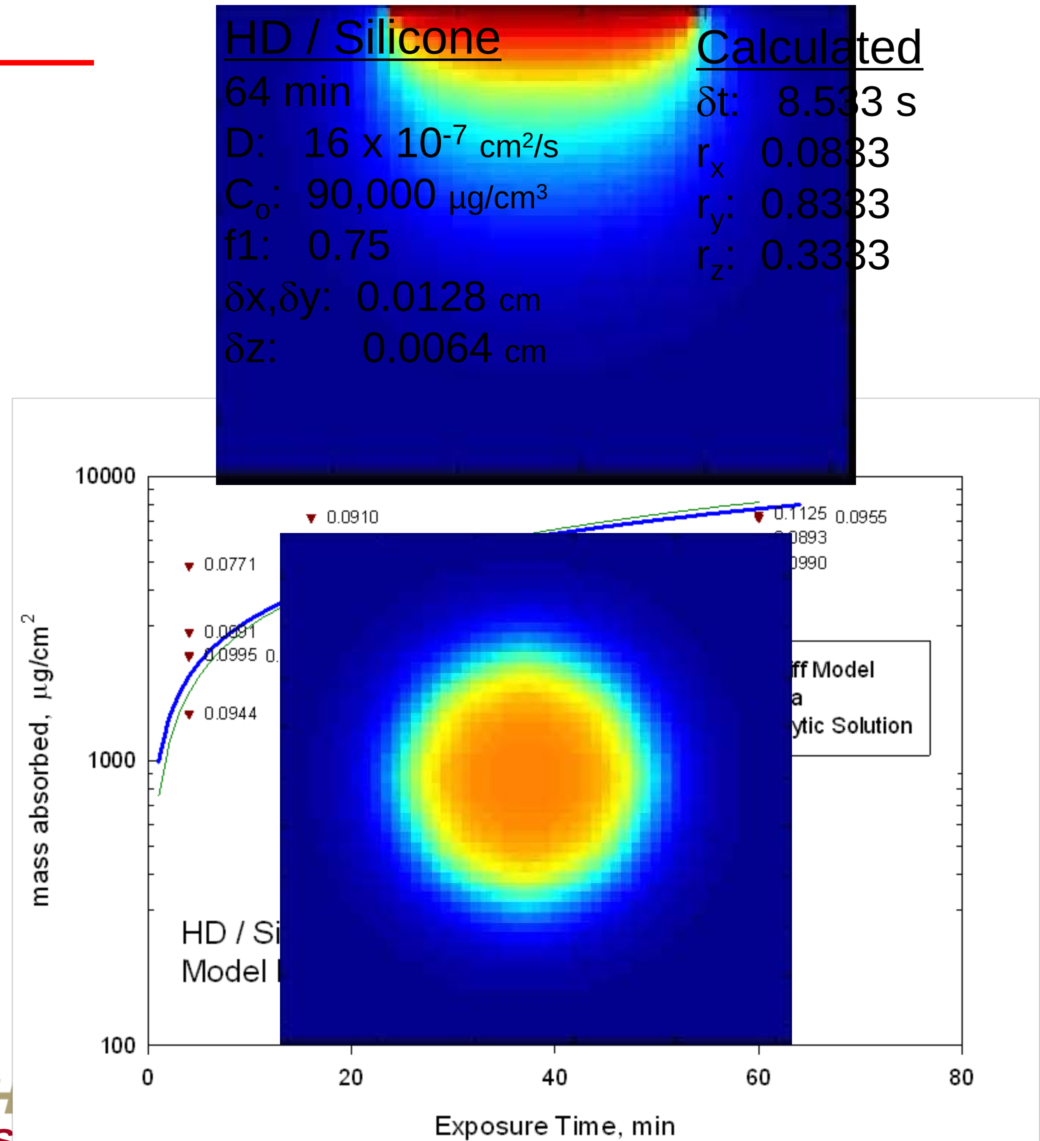


Environmental Conditions (Continuous)

- Temperatures from 10-50 °C
- Relative humidity from 10-80%

Modeling Agent Sorption into Silicone





Finite Difference: Droplet Configuration

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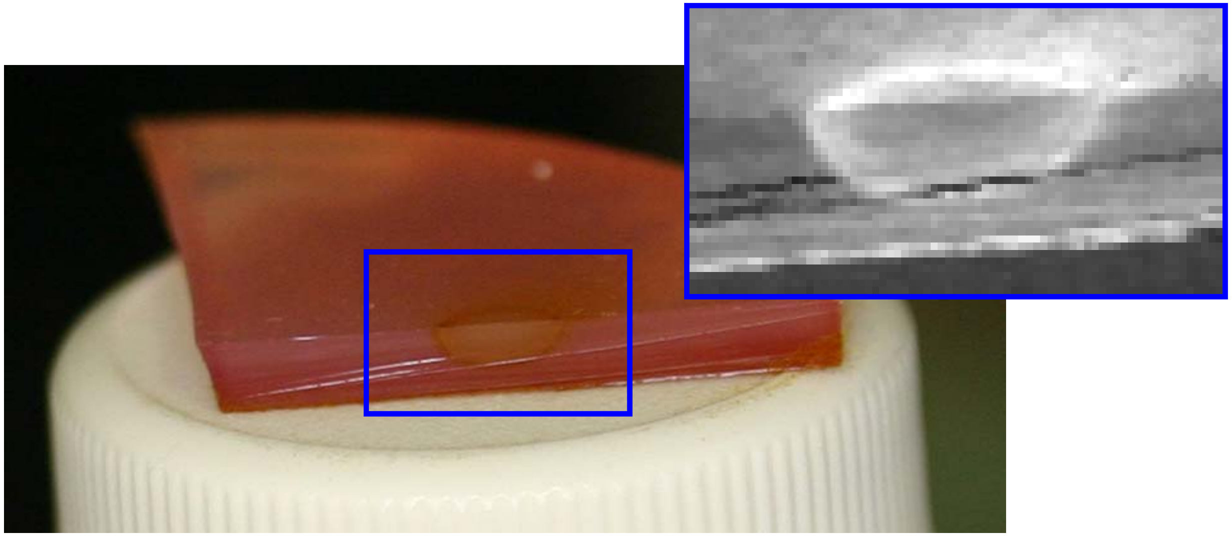
49																							1	1	1	1	1																						

Example of a Drop used for input:

Gray area indicates the drop location on coupon surface.

The drop is positioned on the coupon as specified by the user.

Cross Sectional Imaging



Iodine used as a contrast agent to reveal sorption in silicone
Imaging experiments used to confirm model coefficients (diffusivity and saturation) and methods.

Color Key for Conceptual Model

- Red – deposited agent drop.
- Orange = absorbed agent.
- Dark green – adsorbed agent.
- Blue = adsorbed agent and desorbed agent on surface.
- Purple = decontaminant.
- Green = reaction product.
- Light blue = rinse water.